

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.68e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.96e-01

Confidence level: 4.65e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Metoxuron</div> <div>Measured: 3.45e-05</div> <div>Predicted: 7.34e-06</div>	<div>Image not found</div> <div>Hexaflumuron</div> <div>Measured: 6.30e-05</div> <div>Predicted: 4.80e-08</div>	<div>Image not found</div> <div>2-Methyldecane</div> <div>Measured: 3.00e-07</div> <div>Predicted: 8.09e-01</div>
<div>Image not found</div> <div>Propane, 2-(methylthio)-</div> <div>Measured: 4.85e-06</div> <div>Predicted: 65.7</div>	<div>Image not found</div> <div>MGK-264</div> <div>Measured: 9.68e-06</div> <div>Predicted: 1.19e-05</div>	